Computation of Hypersonic Flow past a Blunt Body in an Inert Binary Gas Mixture in Rotational Non-equilibrium Using the Generalized Boltzmann Equation

Geng Qian[1], Ramesh K. Agarwal[*2], Baoguo Wang[3]

[1,3]Beijing Institute of Technology, Beijing 100081, China; Washington University in St. Louis, Missouri 63130, USA

[1]gloria716@gmail.com; [*2]rka @wustl.edu; [3]bguowang@bit.edu.cn

Abstract

The results of 2-D numerical simulations of hypersonic flow of a single diatomic gas, namely Nitrogen and a binary inert mixture of two gases (which are constituents of air namely N_2, O_2, Ar) past a 2-D blunt body in rotational non-equilibrium from low to high Knudsen Numbers are obtained using the Wang-Chang Uhlenbeck equation or the Generalized Boltzmann Equation. The computational framework available for the classical Boltzmann equation for a monoatomic gas with translational degrees of freedom is extended by including the rotational degrees of freedom in the GBE. The general computational methodology for the solution of the GBE for a diatomic gas is similar to that for the classical Boltzmann equation except that the evaluation of the collision integral becomes significantly more complex due to the quantization of rotational energy levels. There are two main difficulties encountered in computation of high Mach number flows of diatomic gases with rotational degrees of freedom using the GBE: (1) a large velocity domain is needed for accurate numerical description of molecular velocity distribution function resulting in enormous computational effort in calculation of the collision integral and (2) about 50 to 70 energy levels are needed for accurate representation of the rotational spectrum of the gas. These two problems result in very large CPU and memory requirements for shock wave computations at high Mach numbers (>6). A two level Rotational-Translational (RT) relaxation model has been employed to address this problem; as a result, the efficiency of calculations increases by several orders of magnitude. For numerical solution of GBE for an inert binary gas mixture, the GBE is formulated in the impulse space. For numerical solution of GBE for an inert binary gas mixture, the GBE is formulated in the impulse space. The inert binary gas mixtures may consist of both monatomic and diatomic gases with arbitrary concentrations and mass ratios. In particular, the method is applied to simulate two of the three primary constituents of air (N2, O2, Ar) in a binary mixture at 1:1 density ratio and air concentration ratio with gases in translational and rotational non-equilibrium. The results of GBE are compared with DSMC calculations for flow past a blunt body; a reasonably good agreement is obtained. The solutions presented in this paper can also serve as validation test cases for other numerical methods for direct solution of GBE and as an important step towards developing complex 3D simulations for shock waves in a mixture of multiple gases.

Keywords

Generalized Boltzmann Equation; Non-equilibrium Hypersonic Flows; Shock Waves in Inert Gas Mixtures; Rotational and Vibrational Non-equilibrium Flows

Nomenclature

ρ_A = Density of gas A

ρ_B = Density of gas B

m_A =Mass of gas A

m_B = Mass of gas B

d_A = Molecular diameter of gas A

d_B = Molecular diameter of gas B

P_A = Pressure of gas A

P_B = Pressure gas B

U_A = Velocity of gas A

U_B = Velocity of gas B

T_A = Translational temperature of gas A

T_B =Translational temperature of gas B

T_{xA}=Longitudinal component of translational temperature of gas A

T_{xB}=Longitudinal component of translational temperature of gas B

T_{yA}=Transverse component of translational temperature of gas A

T_{yB}=Transverse component of translational temperature of gas B

$T_{rot,\,A}$ = Rotational temperature of gas A

$T_{rot,\,B}$ = Rotational temperature of gas B

$T_{vib,\,A}$ = Vibrational temperature of gas A

$T_{vib,\,B}$ = Translational temperature of gas B

M = Mach number

Kn = *Kn*udsen number

A and B represent Nitrogen (N_2), Oxygen (O_2) or Argon (Ar)

Introduction

In recent years, there has been a resurgence of interest in US Air Force in space access and consequently the hypersonic aerodynamics of its future space operations vehicles, long-range-strike vehicles and military-reusable launch vehicles. The size and weight of a hypersonic vehicle and thus its flight trajectory and required propulsion system are largely determined from aerodynamic considerations. Various positions in the flight envelope of such space vehicles may be broadly classified into the continuum, transition and free molecular regimes. Hence, a need exists for a single unified Computational Fluid Dynamics (CFD) code that can treat all the three flow regimes accurately and efficiently. At an altitude greater than 90 km, the *Kn*udsen number *Kn* is greater than 10, corresponding to the rarefied regime, in which the kinetic model such as DSMC can be used for the simulation. At altitudes under 70 km, *Kn* is small, corresponding to the continuum regime, in which continuum equations namely the Euler or Navier-Stokes equations can accurately and efficiently model the flow field. For altitudes between 70 and 90 km, the *Kn*udsen numbers are in the neighbourhood of unity; and the flow fields fall in the transition regime, for which both the Navier-Stokes equations and DSMC method have significant limitations. Navier-Stokes equations are no longer accurate because of significant departure from equilibrium and DSMC method becomes computationally prohibitive because of large number of particles required for accurate simulations.

A number of alternative approaches have been proposed and investigated in the literature such as the Burnett equations, Grad's moment equations or Eu's equations. These equations collectively are known as the Extended Hydrodynamics (EHD) equations. However, the progress has been limited and furthermore the accuracy of the EHD equations remains questionable because of the asymptotic nature of the Chapman-Enskog expansion (e.g. for the Burnett equations), the issues related to regularization and the difficulty in imposing the exact kinetic boundary conditions on the surface of the body. Physically, gas flows in transition regime, where Kn is O(1), are characterized by the formation of narrow, highly non-equilibrium zones (Knudsen layers) of thickness of the order of molecular mean free path λ; the flow structure is then determined by the fast kinetic processes. Moreover, in case of unsteady flows, an initial Knudsen time interval is of the order $\tau_0 = \lambda/\nu$, where ν is the molecular velocity. Thus, the Knudsen layer can be computed accurately only by directly solving the Boltzmann equation.

Boltzmann equation describes the flow in all the regimes and is applicable for all Knudsen numbers from zero to infinity. In a previous paper, the 2-D Classical Boltzmann Solver (CBS) of Professor Tcheremissine was applied to simulate the flow field due to supersonic flow of a monoatomic gas past blunt bodies from low to high Knudsen Numbers. A conservative discrete ordinate method, which ensures strict conservation of mass, momentum and energy, was applied in the solver. The effect of Knudsen number varying from 0.01 to 10 was investigated for Mach 3 flows past a blunt body. All the Boltzmann solutions at Kn = 0.01 and 0.1 were compared with the Navier-Stokes and augmented Burnett solutions, and the DSMC solutions obtained using the 'SMILE' code of Professor Ivanov. In the Boltzmann and DSMC computations, the gas was assumed to be composed of hard sphere. In the present paper, the work for monoatomic gases has been extended reported in reference to diatomic gases and a binary inert mixture of monoatomic and diatomic gases by solving the GBE.

Boltzmann Equation for Monoatomic, Polyatomic and Inert Mixture of Gases

Classical Boltzmann Equation

The classical Boltzmann equation considers gases without internal degrees of freedom. In other words, the energy states for the molecules in a gas are composed solely of translational energy. As a result, the necessity of considering rotational-translational (RT) relaxations and vibrational-translational (VT) relaxations is eliminated. It is strictly true for monoatomic gases. Therefore, the applicability of the classical Boltzmann equation in simulating rarefied gas flows at high Mach numbers becomes limited since these flows have high temperatures where rotational energy states, and even vibrational energy states of the gas become important. The classical Boltzmann equation in a two-dimensional Cartesian coordinate system can be written as

$$\frac{\partial f}{\partial t}+\xi_x\cdot\frac{\partial f}{\partial x}+\xi_y\cdot\frac{\partial f}{\partial y}=I(f,f)\equiv -L(f,f)+G(f,f) \qquad (1)$$

where *L(f, f)* and *G(f, f)* represent the contributions of a pair of molecules to the change in the distribution function based upon the pre-collision molecular states and the post-collision molecular states respectively.

L(f, f) and *G(f, f)* are given by equation (2) and equation (3) respectively.

$$L(f,f)=\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{b_m} f\cdot f_1\cdot g\cdot b\cdot db\cdot d\varepsilon\cdot d\xi_1 \qquad (2)$$

$$G(f,f)=\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{b_m} f'\cdot f_1'\cdot g\cdot b\cdot db\cdot d\varepsilon\cdot d\xi_1 \qquad (3)$$

In equation (2), f and f_1 represent the pre-collision probabilities for the two molecules undergoing the collision. In equation (3), f' and f_1' represent the post-collision probabilities for the two molecules just after the collision.

Generalized Boltzmann Equation (Wang-Chang-Uhlenbeck Equation)

Non-equilibrium processes in a gas with internal degrees of freedom of molecules can be studied by using the Generalized Boltzmann Equation (GBE) or the Wang-Chang-Uhlenbeck equation (WC-UE), where the internal and translational degrees of freedom are considered in the framework of quantum and classical mechanics respectively. The GBE or WC-UE for a diatomic gas in thermodynamic non-equilibrium can be written in the form:

$$\frac{\partial f_i}{\partial t}+\xi_i\cdot\frac{\partial f_i}{\partial x}=\sum_{j,k,l}\int_{-\infty}^{\infty}\int_{\Omega}(f_k f_l-f_i f_j)g\sigma_{ij}^{kl}d\Omega d\xi_j \qquad (4)$$

In equation (4), $d\Omega=\sin\theta d\theta d\varphi$ is the distribution function, where i is the set of quantum numbers determining the internal state of the molecule; ξ_i is the velocity of the molecule in the ith state; and σ_{ij}^{kl} is the cross section for the collision responsible for this change of the internal states. The static temperature T can be determined from the longitudinal temperature T_{xx} and the transverse temperatures T_{yy} and T_{zz} as given by equation (5):

$$T=\frac{T_{xx}+T_{yy}+T_{zz}}{3} \qquad (5)$$

Classical/Generalized Boltzmann Equation for a Mixture of Gases

To solve the classical Boltzmann equation (CBE) for a mixture of monoatomic gases or the generalized Boltzmann (GBE) equation for a mixture of diatomic gases, these equations are formulated in impulse space. The formulations of CBE and GBE in impulse space are described below.

1) Mixture of Monoatomic Gases

The system of Boltzmann kinetic equations for an inert mixture of monoatomic gases containing several gases can be written in the form

$$\frac{\partial f_i}{\partial t}+\xi_i\frac{\partial f_i}{\partial \mathbf{x}}=\boldsymbol{I}_i, i=1,\ldots,K \qquad (6)$$

The collision integrals I_i have the form

$$I_i=\sum_j\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{b_m}(f_i' f_j'-f_i f_j)gbdbd\varphi d\xi_j, i=1,\ldots,K \qquad (7)$$

In equation (7), b_m is the maximum interaction distance between the molecules, i denotes a particular gas and K denotes the number of gases in the mixture. The following abbreviations have been used:

$$f_i\equiv f_i(\xi_i,\mathbf{x},t),\ f_j\equiv f_j(\xi_j,\mathbf{x},t),$$
$$f_i'\equiv f_i(\xi_i',\mathbf{x},t),,\ f_j'\equiv f_j(\xi_j',\mathbf{x},t) \qquad (8)$$

For construction of the conservative method of evaluation of the collision integrals I_i for a gas mixture one needs to transform equation (6) from velocity variables to the impulse variables defined by the relation $p_i = m_i \xi$, where m_i denotes the molecular mass. Thus, the variables change as:

$$(\xi_i,\mathbf{x},t)\to(\mathbf{p}_i,\mathbf{x},t),\qquad f_i(\xi_i,\mathbf{x},t)\to f_i^*(\mathbf{p}_i,\mathbf{x},t) \qquad (9)$$

From the normalization condition for particle density of gas specie i, one can write

$$\int f_i d\xi=\int f_i^* d\mathbf{p}=n_i \qquad (10)$$

and obtain $f_i^*=m_i^{-3}f_i$ (11)

In the impulse variables, the system of Boltzmann equations takes the form

$$\frac{\partial f_i^*}{\partial t}+\frac{\mathbf{p}_i}{m_i}\frac{\partial f_i}{\partial \mathbf{x}}=\mathbf{I}_i^*,\qquad i=1,\ldots,K \qquad (12)$$

The collision integrals take the form

$$\mathbf{I}_i^*=\sum_j\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{b_m}(f_i^{*'}f_j^{*'}-f_i^* f_j^*)g^* bdbd\varphi d\mathbf{p}_j,$$
$$g^*=\left|\mathbf{p}_j/m_j-\mathbf{p}_i/m_i\right| \qquad (13)$$

2) Mixture of Diatomic Gases

The system of Boltzmann equations for a mixture of diatomic gases can be written by recasting the Wang Chang-Uhlenbeck equations (WC-UE) or the Generalized Boltzmann Equation (GBE) for the mixture in the impulse space. The GBE for a single

gas can be written the velocity space as

$$\frac{\partial f_\alpha}{\partial t}+\xi_\alpha\frac{\partial f_\alpha}{\partial \mathbf{x}} = \sum_{\beta\chi\delta}\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{b_m}(f_\chi f_\delta\omega_{\alpha\beta}^{\chi\delta}-f_\alpha f_\beta)P_{\alpha\beta}^{\chi\delta}g_{\alpha\beta}bdbd\varphi d\xi_\beta \quad (14)$$

In equation (14), the indices α,β,χ,δ denote the energy levels, $\omega_{\alpha\beta}^{\chi\delta}=(q_\chi q_\delta)/(q_\alpha q_\beta)$, in which q_α is the degeneration of the energy level α, $P_{\alpha\beta}^{\chi\delta}$ is the probability of transition from levels α,β to the levels χ,δ, and $g_{\alpha\beta}=\left|\xi_\alpha-\xi_\beta\right|$. For rotational energy levels, $q_\alpha=2\alpha+1$. For vibrational levels, the degeneration is absent and therefore $q_\alpha=1$. It is assumed that the degenerate energy levels are the same for all components of the mixture. The generalization of equation (14) to a mixture of diatomic gases takes the form:

$$\frac{\partial f_{i,\alpha}}{\partial t}+\xi_{i,\alpha}\frac{\partial f_{i,\alpha}}{\partial \mathbf{x}} = \sum_j\sum_{\beta\chi\delta}\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{b_m}(f_{i,\chi}f_{j,\delta}\omega_{\alpha\beta}^{\chi\delta}-f_{i,\alpha}f_{j,\beta})P_{i,\alpha\beta}^{j,\chi\delta}g_{\alpha\beta}bdbd\varphi d\xi_{j,\beta} \quad (15)$$

where subscript i denotes a particular specie and for a mixture of K species, i = 1, 2, …….K. Again to build the conservative method of evaluation of the collision operator on the right hand side of equation (15), the equation is transformed to the impulse space to obtain:

$$\frac{\partial f_{i,\alpha}}{\partial t}+\frac{\mathbf{p}_{i,\alpha}}{m_i}\frac{\partial f_{i,\alpha}}{\partial \mathbf{x}} = \sum_j\sum_{\beta\chi\delta}\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{b_m}(f_{i,\chi}f_{j,\delta}\omega_{\alpha\beta}^{\chi\delta}-f_{i,\alpha}f_{j,\beta})P_{i,\alpha\beta}^{j,\chi\delta}g_{\alpha\beta}bdbd\varphi d\mathbf{p}_{j,\beta} \quad (16)$$

Numerical Method for the Solution of Boltzmann Equation

The details of the numerical method to solve equation (1), the classical Boltzmann equation have been described by Tcheremissine in a number of papers. The methodology to solve equation (4)–the Wang-Chang Uhlenbeck (WU-CE) equation or the Generalized Boltzmann equation (GBE) is described in reference paper again by Tcheremissine who pioneered the direct numerical solution approach for the Boltzmann equation. The methodology to solve the Boltzmann equation for a mixture of monoatomic gases, equation (12) and for a mixture of diatomic gases, equation (16) in impulse space has been described in detail by Agarwal and Tcheremissine. The interested reader can look into these references. 1D, 2D and 3D codes have been developed for solutions of these equations.

Results

1-D Shock Wave Solutions for Binary Gas Mixture of N_2 and Ar, and N_2 and O_2 in Translational and Rotational Non-equilibrium

In a previous paper, the computations were performed for 1D shock structure in a binary inert mixture of monoatomic gases and the code was validated by comparing the results with computations of Kosuge et al.. To solve the GBE to account for both the translational and rotational relaxations, the code was validated by comparing the results against the experimental data of Alsmeyer. The results presented in the following sections have been validated as much as possible by comparing with the DSMC solutions or other numerical solutions available in the literature. The solutions are grid independent; which was ensured by computing solutions on at least two grids.

1) N_2 and Ar Mixture

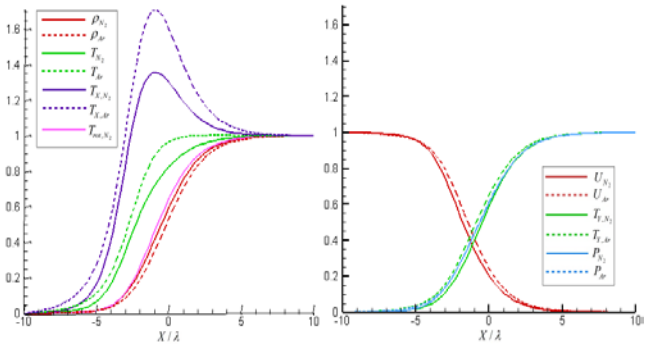


FIG. 1 SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT MACH 2

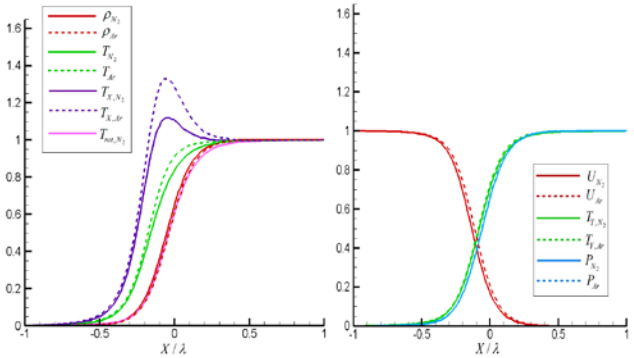


FIG. 2 SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 DENSITY RATIO AT MACH 2

In this case, N_2 is in both the translational and rotational non-equilibrium while Ar is in

translational non-equilibrium only. The mass ratio equals 1.4260 and the diameter ratio equals 0.8356. The gases are assumed to be non-reacting. Figure 1 shows various flow properties for the two gases at Mach 2 with concentration as in air. As shown in Figure 1, N_2 lighter than Ar, experiences changes in the shock properties earlier than Ar. However, it is important to note that the peak of the longitudinal component of the translational temperature for Ar is much higher than that for N_2. This effect is due to transfer of rotational energy of N_2 into the translational energy of Ar. Figure 2 shows various flow properties for the two gases at Mach 2 with 1:1 density ratio. Again the behavior of change in shock properties is the same as that in Figure 1 except that the peaks of normalized longitudinal temperatures of the two gases are smaller than those in Figure 1 as expected.

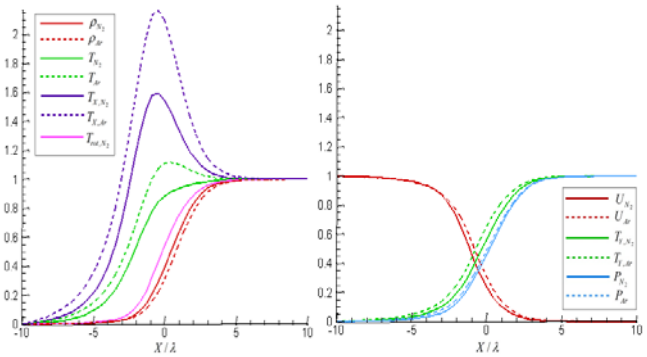


FIG. 3 SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT MACH 5

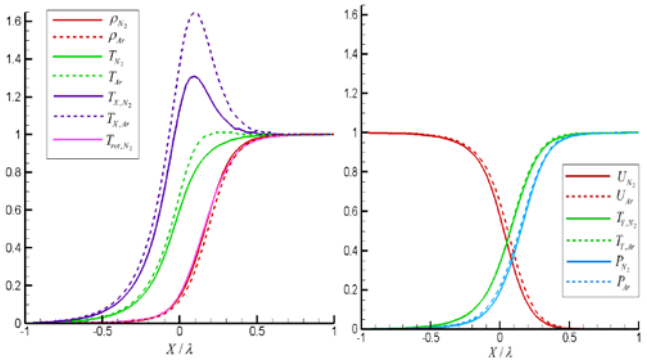


FIG. 4 SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 DENSITY RATIO AT MACH 5

Figures 3 and 4 show various flow properties for the two gases at Mach 5 with concentration as in air and for a density ratio of 1:1 respectively. These figures are similar to Figures 1 and 2 in terms of variation of flow properties of the two gases across the shock. However due to higher Mach number, the peaks of normalized longitudinal temperatures and translational temperature of the two gases are much higher and there is greater transfer of rotational energy of Nitrogen into translational energy of Argon.

2) *N_2 and O_2 Mixture*

In this case, the mixture of N_2 and O_2 are in both translational and rotational non-equilibrium. The mass ratio equals 1.1423 and the diameter ratio equals 0.9156. The gases are again assumed to be non-reacting. Figure 5 shows various flow properties for the two gases across the shock at Mach 2 for air concentration ratio. Again as before in Figure 1, N_2 lighter than O_2, experiences changes in the shock properties earlier than O_2. However, it is important to note that the peak of the longitudinal component of the translational temperature for O_2 is only slightly higher than that for N_2 in this case compared to that in Figure 1 where peaks of normalized longitudinal temperature and translational temperature for Ar have much higher value than that for N_2. It is due to the fact that the mass and diameter ratio of N_2 and O_2 are nearly the same; therefore there is little transfer of energy between the two in the mixture. Figure 6 shows various flow properties for the two gases across the shock at Mach 2 for 1:1 density ratio. Compared to Figure 5, the peaks for the longitudinal component of translational temperature are higher in this case as expected. Figure 7 and 8 show various flow properties for the two gases across the shock at Mach 5 for air concentration ratio and 1:1 density ratio respectively. Again the results are similar to those shown in Figures 5 and 6 except that the peaks for longitudinal component of translation temperature as well as translation temperature are much higher because of greater Mach number.

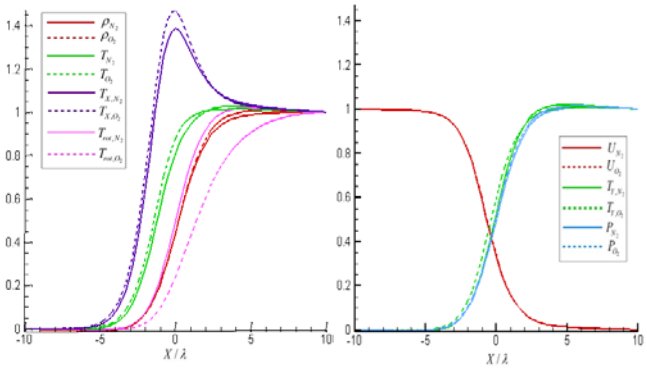


FIG. 5 SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT MACH 2

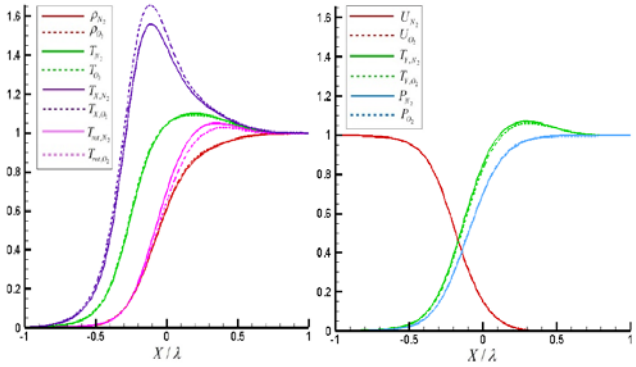


FIG. 6 SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 DENSITY RATIO AT MACH 2

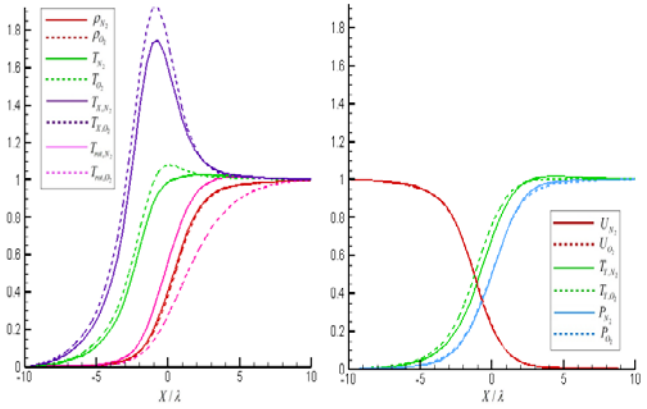


FIG. 7 SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT MACH 5

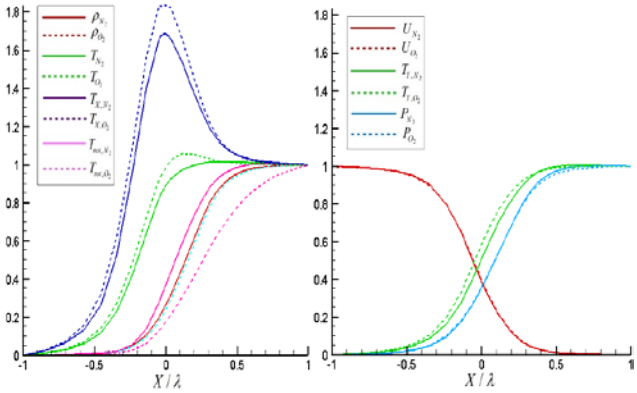


FIG. 8 SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 DENSITY RATIO AT MACH 5

Flow of Nitrogen past a 2D Blunt Body at High Mach Numbers

Figure 9 shows a 2D blunt body and Figure 10 shows a typical Cartesian grid around the blunt body. The flow of nitrogen past the blunt body at M = 3 and Kn varying from 0.1 to 10 are taken into consideration. The far field temperature in the free stream is 205 K and the body temperature is 700 K.

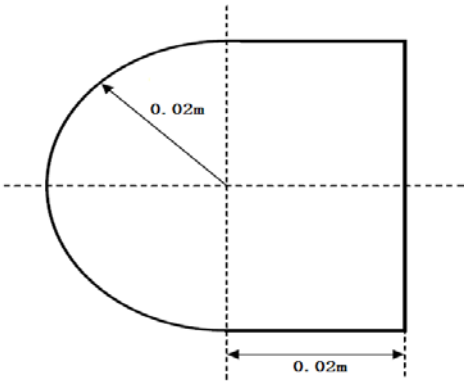


FIG. 9 GEOMETRY OF 2D BLUNT BODY

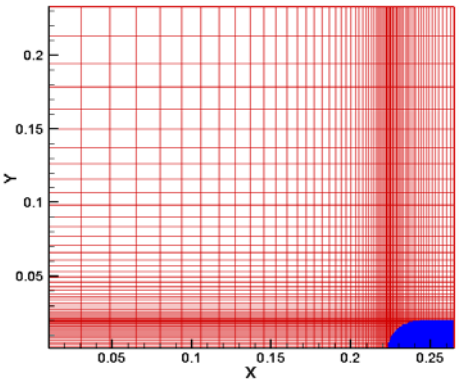
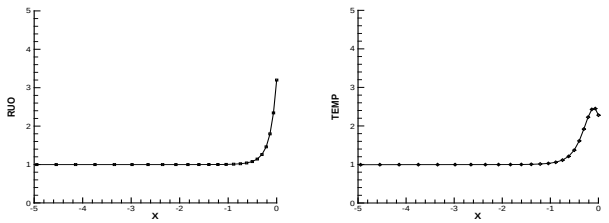
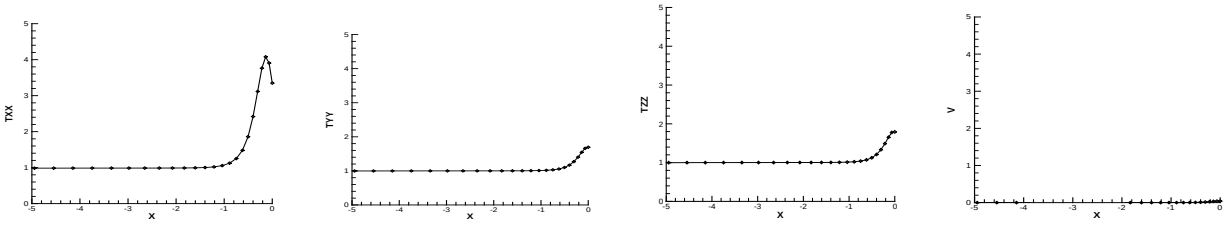


FIG. 10 CARTESIAN GRID AROUND THE BLUNT BODY

Figures 11-16 show the results of computations for flow of Nitrogen past the blunt body in both translational and rotational non-equilibrium at M = 3 at Kn = 0.1, 1.0 and 10. Both the variations in flow quantities such as density, u- and v-components of velocities, total temperature, rotational temperature, and x-, y-, and z-components of translational temperature as well as the contour plots of these quantities in the computational domain are shown. These results indicate the predominant effect of rotational degrees of freedom on the flow field.

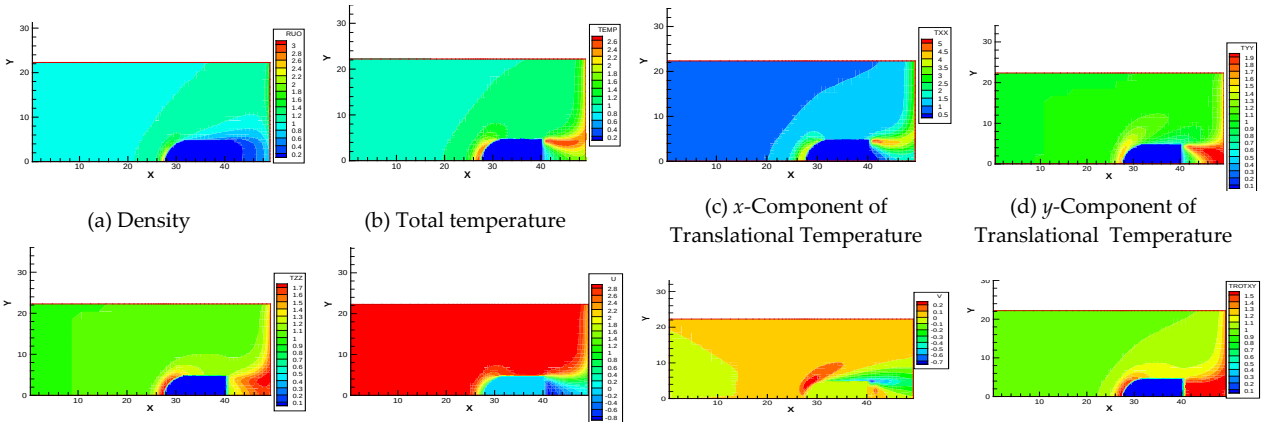


(a) Density (b) Total Temperature (c) u-Component of Velocity (d) Rotational Temperature



(e) x-Component of Translational Temperature (f) y-Component of Translational Temperature (g) z-Component of translational (h) v-Component of Velocity Temperature

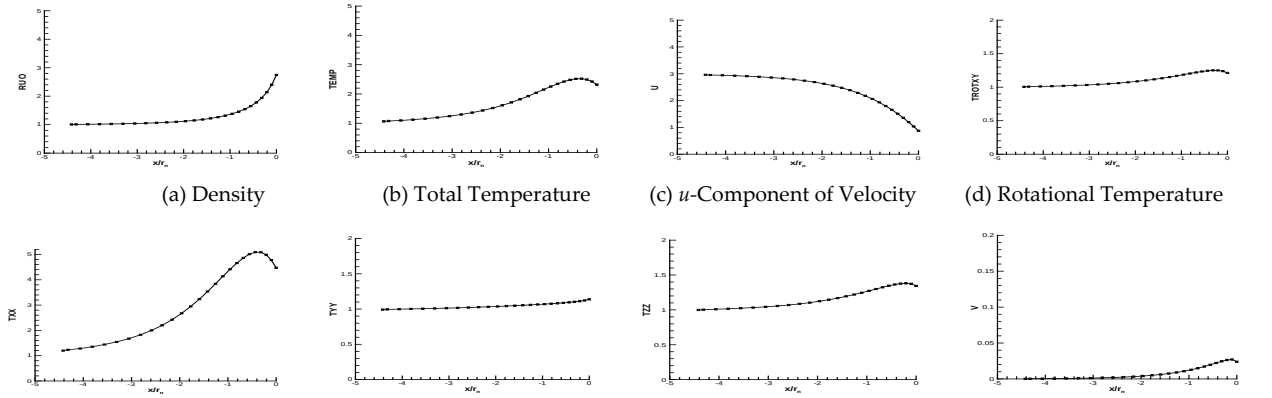
FIG. 11 DISTRIBUTIONS ALONG THE STAGNATION STREAMLINE OF THE BLUNT BODY, $M = 3$, $Kn = 0.1$



(a) Density (b) Total temperature (c) x-Component of Translational Temperature (d) y-Component of Translational Temperature

(e) z-Component of Translational Temperature (f) u-Component of Velocity (g) v-Component of Velocity (h) Rotational Temperature

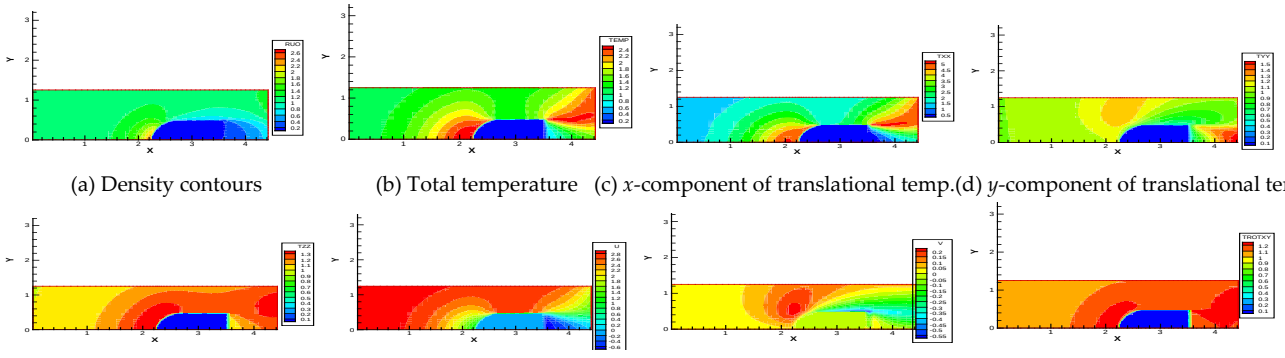
FIG. 12 FLOW FIELD CONTOURS FOR NITROGEN FLOW PAST A BLUNT BODY, $M = 3$, $Kn = 0.1$



(a) Density (b) Total Temperature (c) u-Component of Velocity (d) Rotational Temperature

(e) x-Component of Trans. Temp. (f) y-Component of Trans. Temp (g) z-Component of Trans. Temp. (h) v-component of Velocity

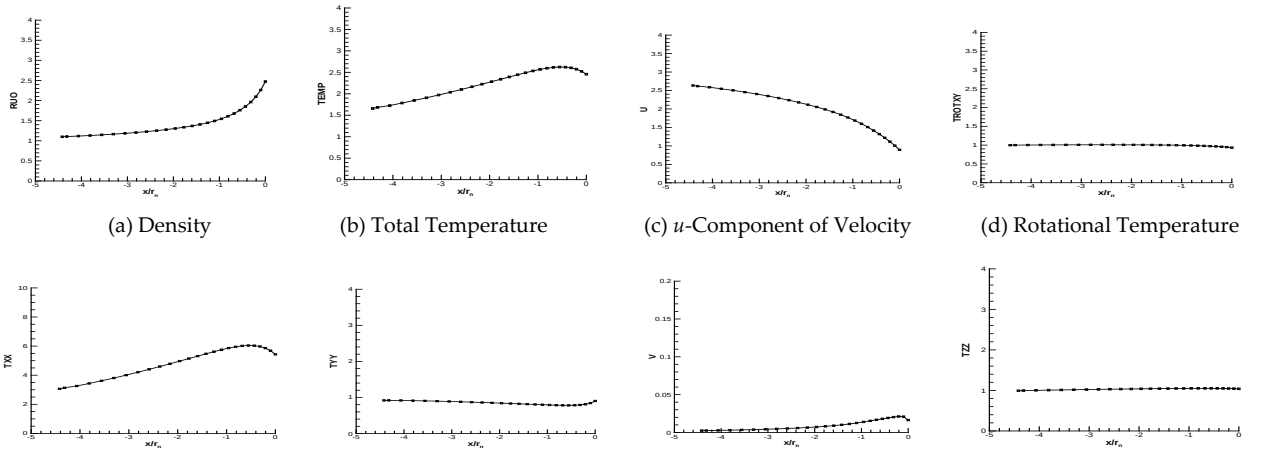
FIG. 13 DISTRIBUTIONS ALONG THE STAGNATION LINE OF THE BLUNT BODY, M =3, $Kn = 1.0$



(a) Density contours (b) Total temperature (c) x-component of translational temp. (d) y-component of translational temp.

(e) z-component of translational temp. (f) u-component of velocity (g) v-component of velocity (h) Rotational temperature

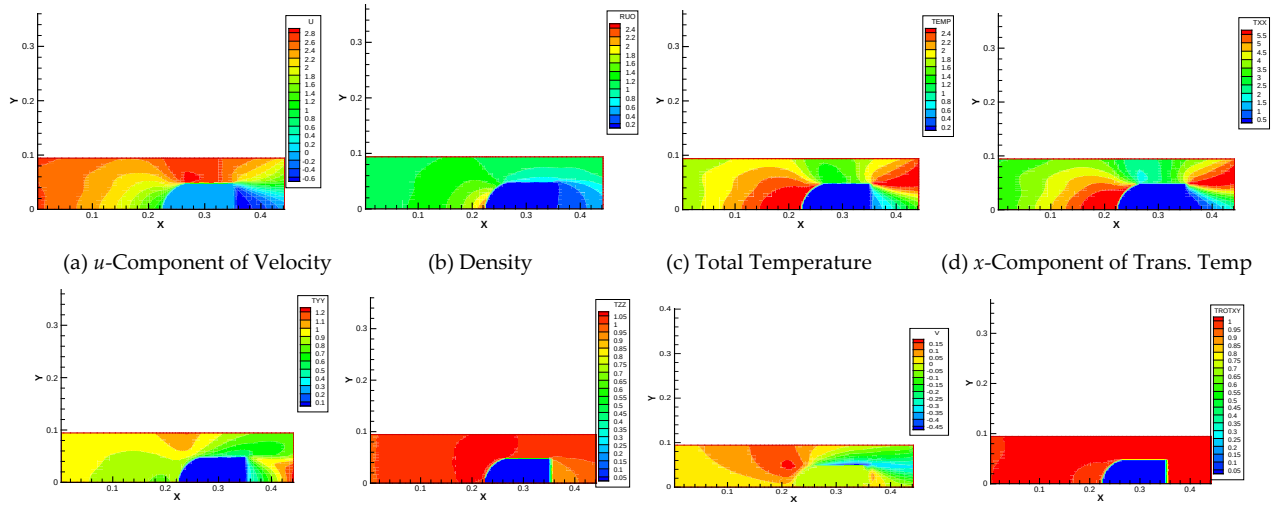
FIG. 14 FLOW FIELD CONTOURS FOR FLOW OF NITROGEN PAST A BLUNT BODY, $M = 3$, $Kn = 1.0$



(a) Density (b) Total Temperature (c) *u*-Component of Velocity (d) Rotational Temperature

(e) x-Component of Trans. Temp. (f) y-Component of Trans. Temp. (g) z-Component of Trans. Temp. (h) v-Component of Velocity

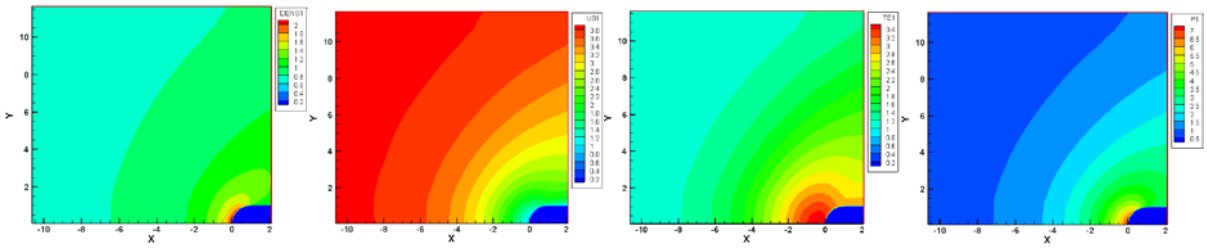
FIG. 15 DISTRIBUTIONS ALONG THE STAGNATION STREAMLINE OF THE BLUNT BODY, M = 3, Kn = 10



(a) *u*-Component of Velocity (b) Density (c) Total Temperature (d) *x*-Component of Trans. Temp

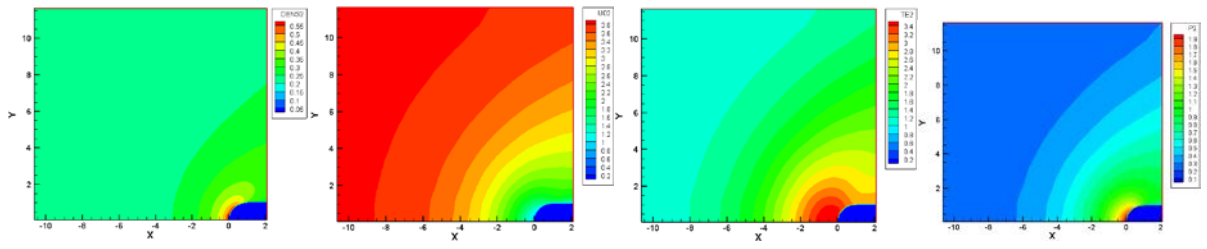
(e) y-Component of Trans. Temp. (f) *z*-Component of Trans. Temp. (g) *v*-Component of Velocity (h) Rotational Temperature

FIG. 16 FLOWFIELD CONTOURS FOR FLOW OF NITROGEN PAST A BLUNT BODY, M =3, Kn = 10



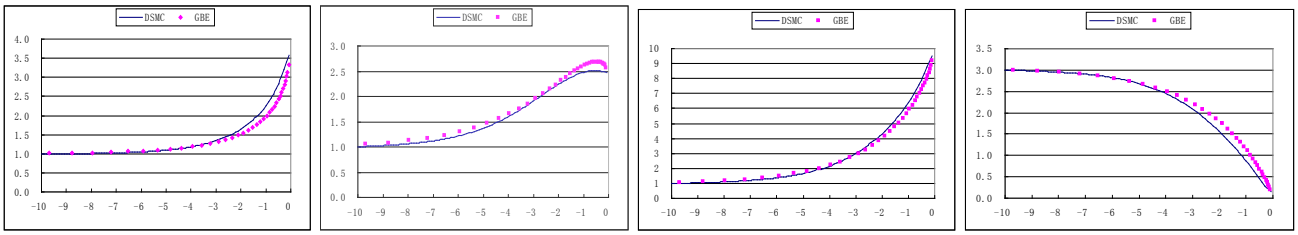
(a) Density Contours (b) x-Component of Velocity (c) Total Temperature Contours (d) Pressure Contours

FIG. 17 FLOWFIELD CONTOURS OF N_2 IN THE N_2-O_2 GAS MIXTURE PAST A BLUNT BODY, M =3, Kn = 1



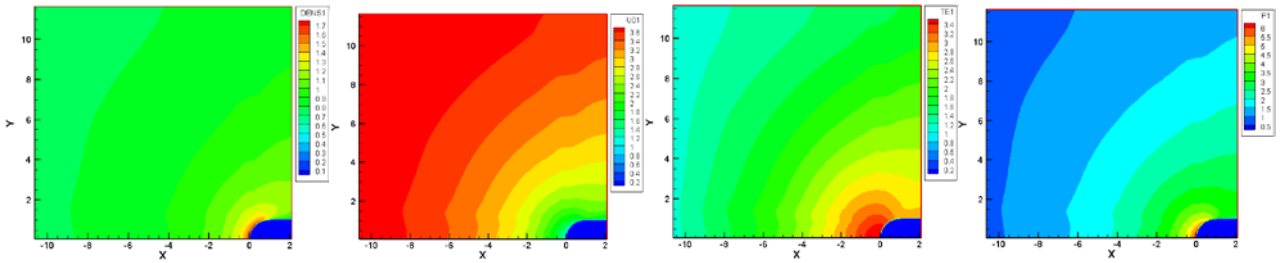
(a) Density Contours (b) x-Component of Velocity (c) Total Temperature Contours (d) Pressure Contours

FIG. 18 FLOWFIELD CONTOURS FOR O_2 IN THE N_2-O_2 GAS MIXTURE PAST A BLUNT BODY, M = 3, Kn = 1



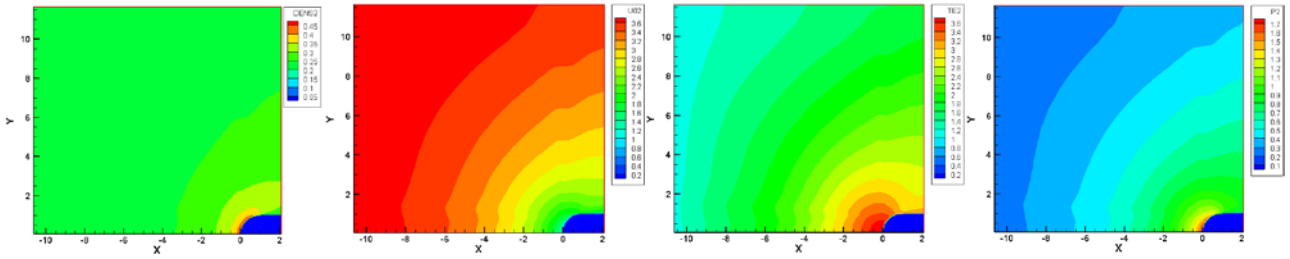
(a) Density (b) Total Temperature (c) Pressure (d) Mach Number

FIG. 19 COMPARISON OF DSMC AND GBE RESULTS FOR N_2 IN THE N_2-O_2 GAS MIXTURE FLOW PAST A BLUNT BODY, M = 3, Kn = 1



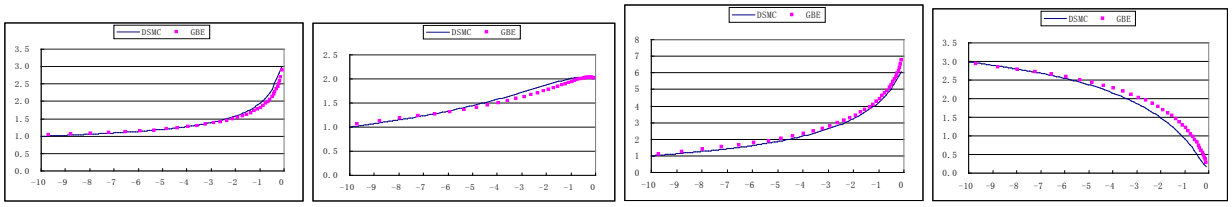
(a) Density Contours (b) x-Component of Velocity (c) Total Temperature Contours (d) Pressure Contours

FIG. 20 FLOWFIELD CONTOURS FOR N_2 IN THE N_2-O_2 GAS MIXTURE PAST A BLUNT BODY, M =3, Kn = 3



(a) Density Contours (b) x-Component of Velocity (c) Total Temperature Contours (d) Pressure Contours

FIG. 21 FLOWFIELD CONTOURS FOR O_2 IN THE N_2-O_2 GAS MIXTURE PAST A BLUNT BODY, M =3, Kn = 3



(a) Density (b) Total Temperature (c) Pressure (d) Mach Number

FIG. 22: COMPARISON OF DSMC AND GBE RESULTS FOR N_2 IN THE N_2-O_2 GAS MIXTURE FLOW PAST A BLUNT BODY, M =3, Kn = 3

Flow of Mixture of Nitrogen and Oxygen past a 2D Blunt Body at High Mach Numbers

Figures 17 and 18 show the results of computations for flow of N_2 and O_2 mixture past a blunt body in both translational and rotational non-equilibrium at Mach 3 and Kn = 1. The contours plots of various flow quantities are shown for both N_2 and O_2 in the mixture of N_2 and O_2. Figure 19 shows the excellent agreement between GBE results and DSMC Figures 20 and 21 show the results of computations for flow of N_2 and O_2 mixture past a blunt body in both translational and rotational non-equilibrium at Mach 3 and Kn = 3. Figure 22 shows the excellent agreement between GBE results and DSMC method. These comparisons validate the GBE code for a mixture of gases in translational and rotational non-equilibrium.

Conclusions

The direct method of Tcheremissine has been applied to solve the Generalized Boltzmann Equation (GBE) in impulse space for computation of shock waves in a binary mixture of non-reacting monoatomic and diatomic gases in translational and rotational non-equilibrium. The GBE solver has been validated by computing the 1D shock structure in Nitrogen and comparing the results with the experimental data of Alsemeyer. The binary gas mixture code was validated by comparing the results with the computations of

Kosuge et al.. The 1-D binary gas mixture code has been employed to compute the 1D shock structure in binary gas mixtures (N_2-Ar and N_2-O_2) for Rotational-Translational (R-T) relaxations. The 2-D solver has been exercised successfully to compute the flow field of Nitrogen past a 2D blunt body in both translational and rotational non-equilibrium and has been validated by comparing the computations with the results of DSMC method. Good agreement between the two solutions has been obtained.

REFERENCES

Agarwal, R. K. and Tcheremissine, F.G., "Computation of Hypersonic Shock Wave Flows of Diatomic Gases and Gas Mixtures Using the Generalized Boltzmann Equation," AIAA Paper 2010-813, 48th AIAA Aerospace Sciences Meeting Including the New Horizons Forum and Aerospace Exposition, Orlando, Florida, 4-7 January 2010.

Alsmeyer, H., "Density Profiles in Argon and Nitrogen Shock Waves Measured by the Absorption of an Electron Beam," J. of Fluid Mechanics, 74 (1976): 497-513.

Beylich, A.A, "An Interlaced System for Nitrogen Gas," Proc. of CECAM Workshop, ENS de Lyon, France, 2000.

Bird, G.A., Molecular Gas Dynamics and the Direct Simulation of Gas Flows, New York: Oxford Science Publications, 1994.

Burnett, D., "The Distribution of Velocities and Mean Motion in a Slight Non-Uniform Gas," Proc. of the London Mathematical Society, 39 (1935): 385-430.

Chapman, S. and Cowling, T.G., The Mathematical Theory of Non-Uniform Gases, New York: Cambridge University Press, 1970.

Chen, R., Agarwal, R.K., and TCheremissine, F.G., "A Comparative Study of Navier-Stokes, Burnett, DSMC, and Boltzmann Solutions for Hypersonic Flow Past 2-D Bodies," AIAA Paper 2007-0205, 2007.

Eu, B.C., Kinetic Theory and Irreversible Thermodynamics, New York: John Wiley, 1992.

Grad, H., "On the Kinetic Theory of Rarefied Gases," Comm. Pure App1. Math., 2 (1949): .325-331.

Ivanov, M.S. and Gimelshein, S.E., "Computational Hypersonic Rarefied Flows," Annu. Rev. Fluid Mech., 30 (1998): 469-505.

Kosuge, S., Aoki, K. and Takata, S., "Shock-Wave Structure for a Binary Gas mixture: Finite-Difference Analysis of the Boltzmann equation for Hard-Sphere Molecules," European Journal of Mechanics B – Fluids, 20 (2001): 87-126.

Oran, E.S., Oh, C.K., and Cybyk, B.Z., "Direct Simulation Monte Carlo: Recent Advances and Application," Annu. Rev. Fluid Mech., 30 (1998): 403-441.

Tcheremissine, F. G., Agarwal, R.K. and Wilson, C.D, "A Two-level Kinetic Model for Rotational- Translational Relaxations in a Diatomic Gas," AIAA Paper 2008-3932, 38th AIAA Fluid Dynamics Conference, Seattle, Washington, 23-26 June 2008.

Tcheremissine, F. G., "Conservative Evaluation of Boltzmann Collision Integral in Discrete Ordinates Approximation," Computers and Mathematics with Applications, 35 (1998): 215-221.

Tcheremissine, F. G., "Solution of the Boltzmann Kinetic Equation for High Speed Flows of a Rarefied Gas," Proc. of the 24th Int. Symposium on Rarefied Gas Dynamics, Bari, Italy, 10-16 July, 2004.

Tcheremissine, F.G., "Solution of the Wang Chang – Uhlenbeck Master Equation," Doklady Physics, 47 (2002): 872-875.

Wilson, C. D., Agarwal, R. K. and Tcheremissine, F. G.., "Computation of Hypersonic Shock Waves in Inert Gas Mixtures Using the Generalized Boltzmann Equation," AIAA Paper 2011-3134, AIAA 42nd Thermophysics Conference, Hawaii, 27-30 June 2011.